MODELING THE S$_2$ FLUORESCENCE SPECTRA OF COMETS. D. C. Boice, Southwest Research Institute, San Antonio TX 78228-0510, USA, DBoice@swri.edu, C. Laffont, Observatoire de Besancon, 25010 Besancon, France.

Sulphur-bearing compounds have been detected in many comets; however, a complete accounting of the sulphur budget for parent species in cometary volatiles and dust has not been made. The species, CS, H$_2$S, S$_2$, and S, have been observed in comets prior to the recent apparition of Comet Hyakutake (see, e.g., Feldman [1991]). Observations made at the time of closest approach of Comet Hyakutake revealed the newly discovered species, OCS, with other S-bearing species, S$_2$ (Weaver et al. [1996]; Laffont et al. [1996]), CS, S, and H$_2$S. More complex S-bearing species have been searched for without success and the connection of S compounds with the grains is largely unknown but the atomic abundance of sulphur in Comet Halley's dust was enhanced relatively to solar values (Jessberger and Kissel [1991]). The inventory of sulphur species in comets is relevant to questions regarding the origins of comets and, as sulphur is important biologically, also to the origins of life.

The molecule S$_2$, having a short lifetime, is concentrated in the inner-most region of the coma. To be detected from an Earth-bound satellite, it must be emitted by a comet that closely approaches the Earth. The S$_2$ molecule was first discovered surrendipitously in Comet IRAS-Araki-Alcock at its closest approach to Earth ($\Delta = 0.032 AU$) by A'Hearn et al. [1983a] with an abundance of about 0.1% relative to water. The spectral lines completely disappeared shortly thereafter indicating an outburst had taken place. Krishna Swamy and Wallis [1987] have claimed evidence of S$_2$ in IUE spectra of several comets but their results have been contested (Feldman [1991]).

With its close approach to the Earth ($\Delta = 0.1 AU$), the detection of S$_2$ in Comet Hyakutake could be reasonably expected. A successful detection of S$_2$ using HST on April 1, 1996, at a level of about 0.01% relative to water was reported by Weaver et al. [1996]. Laffont et al. [1996] report the possible detection of S$_2$ in Comet Hyakutake with IUE spectra five days prior to the HST observations on March 27.

We calculated synthetic fluorescence spectra of the $B^3\Sigma_u^-$ — $X^3\Sigma_g^-$ system of S$_2$, by solving the evolution equation of the population of the vibrational levels as a function of time. Let us call n_i the population of the vibrational level i. The temporal evolution of n_i is governed by the following equation:

$$\dot{n}_i = -n_i \sum_j P_{ij} + \sum_j n_j P_{ji}$$

where P_{ij} is the transition probability between i and j. P_{ij} may be either A_{ij} in emission or $B_{ij}\rho_{ij}$ in absorption. The P_{ij} probabilities were calculated using the Franck-Condon factors from Anderson et al. [1979], the absolute lifetimes from Quick and Weston [1981], and the solar irradiance from A'Hearn et al. [1983b]. We took into account the Swings effect due to the heliocentric velocity of the comet. The initial distribution is obtained with a Boltzmann temperature of 208 K, which is a typical temperature of the expanding gas at the surface of the nucleus predicted by coma models (Boice and Benkhoff [1996]).

The model molecule contained 45 levels in the $B^3\Sigma_u^-$ — $X^3\Sigma_g^-$ system of S$_2$. The problem is to solve 45 rate equations in the coupled network of ordinary differential equations, subject to the constraint of a conservation equation. Therefore, the problem is overdetermined and one of the equations is redundant. In practice, we solve the complete set of equations and use the conservation equation to check the accuracy of the solution. The system is solved by using the Gear method (Gear [1971]) for stiff differential equations where time constants vary by many orders of magnitude. This method uses variable time steps and error control techniques to preserve accuracy during the integration. Global linear invariants are found to be conserved approximately to machine accuracy.

Our method is quantitatively different from the multi-cycle fluorescence approach used by Kim et al. [1990]. At no time do we assume that a given level is in steady state. This allows us to calculate the spectrum at very short times (microseconds) up to the point where steady state is achieved.

Synthetic fluorescence spectra of S$_2$ have been calculated as a function of time after release from the nucleus. They are convoluted with a Gaussian of 1.1 nm FWHM to facilitate comparison with IUE spectra. The g-factors for different bands of S$_2$ between 280 and 306 nm are similar to those calculated by Kim et al. [1990] in the case of steady state. An immediate difference is noted between our results and those of Kim et al. [1990]. They argue that the "first-cycle" spectra is achieved only after about 100 seconds. We find that this spectrum is found after a few seconds. This is likely to have implications on the estimated time to achieve steady state of about 500 seconds that Kim et al. [1990] find. We find that a spectrum closely ressembling steady state is reached after 700 s.

To determine the abundance of a molecule, it is necessary to know its scale length, which is related to its lifetime and to the outflow velocity of the gas. Gas dynamics models (see, e.g., Huebner et al. [1990]) give an average outflow velocity of about 0.8 km/s in the inner coma. The lifetime of S$_2$ is not well known. Two estimates of the lifetime have been reported in the literature: $\tau = 250s$ calculated by de Almeida and Singh [1986] and $\tau = 450s$ derived from the detection of S$_2$ in Comet Iras-Araki-Alcock (A'Hearn et al. [1983a], Budzien and Feldman [1992]). We have neglected the role of the collisions on the S$_2$ fluorescence spectra, UV optical depth in the inner coma, and the rotational levels in the calculation of the fluorescence spectrum of S$_2$. Our next step is to investigate the importance of these effects and our revised time to steady state on the scale length and abundance of S$_2$ in Comets Hyakutake and IRAS-Araki-Alcock.

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